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Synthesis, spectral characterization and theoretical studies of some biomedically potent transition metal complexes as possible photocatalyst and DNA cleaver/binder probes

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Synthesis and structural characterization of new coordination complexes has always been a challenging task to the chemists. 3d-metal complexes derived from Schiff bases and their derivatives have been studied extensively due to their facile synthesis, unusual configurations, and structural labiality. The development of such types of complexes as multifunctional materials represents one of the main targets for their potential applications in photocatalyst and DNA clever/binder agents. The Schiff base ligands and their complexes have been synthesized by reported refluxing/condensation method. To establish and confirm the chemical structure of synthesized products, various techniques have been employed viz. FTIR, ^{1}H-NMR, mass spectrometry, electronic, CV, thermal, XRD, SEM-EDX and single crystal X-ray diffraction studies. The useful information about molecular structure and related properties of the synthesized compounds has been produced at B3LYP level using density functional theory. Such complexes have been used as a precursor to fabricate metal oxide nanoparticles by pyrolytic method. The nanoparticles have been characterized by powder X-ray diffraction, SEM, TEM, FT-IR spectroscopy and UV-Vis spectroscopy techniques. The visible light driven photocatalytic activity of prepared nanoparticles has been demonstrated using methylene blue (MB) as a representative dye. DNA offers several potential binding sites for transition metals, including the anionic phosphate backbone, electron-rich bases, and the major or minor grooves. The interaction of synthesized complexes with calf thymus DNA (ct DNA) has been investigated *in vitro* using UV-Vis, fluorescence, CV and gel electrophoresis techniques. The calculated binding constant and site size binding shows the interactive model between complexes and ct DNA. The interaction between plasmid DNA (pTZ57R DNA) and these complexes is confirmed by gel electrophoresis studies. The computer-aided molecular docking techniques have also been carried out to ascertain the mode of action toward the molecular target DNA for selected ligand and complexes.

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Quality by Design (QbD), advances in pharmaceutical technology

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Despite continuous innovations in the pharmaceutical industry for developing futuristic new drug products, there has been a repeated set back owing their low quality and manufacturing standards. The studies and tests required to deliver a new drug to patients last up to 15 years, and cost over 800 million $. Even after a drug is invented, its development may fail due to the proven impossibility of its safe manufacture in a large scale and incompliance with the relevant specifications. The length of the approval process and the requirement to start over for a development cycle of any changes due to the stalemates, even product is licensed has led to concerns for many decades. With the consequent growing concerns and criticism, in this regard, in 2002, the current Good Manufacturing Processes (cGMP) was introduced to improve and modernize the rules that regulate the drug manufacturing and quality. Subsequently, in 2005, the guideline Q8 of the International Conference on Harmonization (ICH), which focused on the content of the Module 3.2.P.2 of the Common Technical Document (CTD), was published. The ICH instituted a series of quality guidelines all emphasizing the adoption of systematic principles of Quality by Design (QbD) and Process Analytical Techniques (PAT). QbD is a patient-centric science and risk-based approach for developing drug products with better understanding of the product(s) and process(es) by planning quality at first hand in order to avoid quality crisis and using the knowledge obtained during the life-cycle of the product to work on a constant improvement. Implementation of QbD-based strategies in pharmaceutical development would provide excellence and significant time shortening in product development, and enormous flexibility in regulatory compliance. It has been emphasized before if the principles described in the ICH Q8, Q9 and Q10 guidelines are implemented together in a holistic manner, this provides an even greater assurance that the patient will receive product that meets the critical quality attributes.

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